Perfect state transfer in networks of arbitrary topology and coupling configuration

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A general formalism of the problem of perfect state transfer is presented. We show that there are infinitely many Hamiltonians which may provide solution to this problem. In a first attempt to give a classification of them we investigate their possible forms and the related dynamics during the transfer. Finally, we show how the present formalism can be used for the engineering of perfect quantum wires of various topologies and coupling configurations.

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I. INTRODUCTION

The faithful transfer of a quantum state between two distant but specified components of a quantum computer is one of the main requirements for practical quantum computation [1]. The two components (e.g., small quantum processors) are typically parts of a larger quantum network and connected via a quantum channel (wire). The state transfer is achieved by converting a stationary information carrier (qubit) to a movable ("flying") one at the input of the wire [1]. The flying qubit is then transmitted through the wire towards its other end where it is converted back into a stationary qubit.

In general, photons are excellent flying qubits as they can be transmitted coherently over very large distances [2]. Hence, many discussions in the field of quantum computing consider that the state to be transmitted is first imprinted onto a photon which is used as the flying qubit over an optical fiber. Clearly, the implementation of such an idea requires a perfect interface between optical systems and the main hardware of the quantum computer. However, such an interface is not always an easy task to realize as the quantum hardware may be based on atoms, ions, molecules or solid state systems, for example. Hence, for short-distance communication (e.g., between two quantum processors) it is desirable to develop new systems which are fully compatible with the quantum hardware and, in addition, are suitable for faithful state transfer.

From the point of view of quantum control the problem under consideration can be rephrased as follows. Given a set of prescribed elements and gates one has to structure a system realizing faithful state transfer for arbitrary input states. Elements of quantum information processing are typically quantum mechanical objects (e.g., ions, quantum dots, Josephson junctions, etc) arranged to form linear chains or planar structures with bipartite interactions which can be manipulated by certain control parameters. Manipulating the strength of the interaction between the quantum elements one can design different types of interactions for the whole system and perform certain gate sequences.

Quantum wires based on systems of permanently coupled quantum objects are of particular interest as they require minimal external control thus avoiding significant errors due to the application of multiple operations (gates) and/or measurements on various sites of the channel. The design of such a kind of *passive* quantum wires and the problem of faithful state transfer have attracted considerable interest over the last years. It was immediately realized, however, that faithful state transfer is not an easy task, even in the absence of dissipation or dephasing, due to the dispersion of the quantum information along the wire. Thus, various methods have been proposed to partially circumvent this problem and to improve the fidelity of the transfer [3, 4, 5, 6, 7, 8, 9, 10].

Throughout this work we focus on *perfect* state transfer over passive quantum wires. So far, the existence of perfect passive quantum wires has been demonstrated in the context of coupled harmonic oscillators [11, 12], arrays of quantum dots [13] and spin chains [10, 14, 15, 16]. The key idea is the engineering of certain coupling configurations (and thus interactions) along the chain which are able to suppress possible dispersion effects and enforce the complete refocus of the transmitted quantum information at the ends of the chain at well defined instants of time. Nevertheless, the majority of these investigations mainly focus on centrosymmetric (also known as mirror symmetric) linear chains while the Hamiltonian characterizing the quantum wire involves nearest-neighbour (NN) interaction only. As a result, they are not applicable to realistic setups where these assumptions are relaxed (e.g., beyond NN couplings) [9], and the design of new perfect quantum wires is necessary [17]. In the worst case scenario where such a design is not feasible, numerical optimisation techniques may be invoked for improvement of the fidelity of the transfer. An alternative solution to this problem relies on the use of the so-called dual-rail encoding involving two nearly identical quantum channels [18]. However, in this case the state transfer does not occur at well defined time instants and

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thus the arrival of the state can be revealed by means of measurements only.

The purpose of this paper is manifold. First we aim to solve the problem of perfect state transfer (PST) in a much broader context. More precisely, we want to investigate the possible forms that the system's Hamiltonian may take to be suitable for PST. In contrast to previous work in the field, here we do not set any *a priory* restrictions to the topology of the system and the configuration of couplings between different sites of the channel. Hence, irrespective of topology and coupling configuration, we show that there are infinitely many Hamiltonians which are suitable for PST. For the sake of illustration, we demonstrate that certain Hamiltonians previously discussed in the literature can be obtained in the framework of our unified theory by setting certain restrictions and using the right parameterisation. Second, we show that our approach provides new ways for quantum wire engineering for systems of arbitrary topology and interactions beyond nearest neighbours, thus generalising existing work in this context [15, 16, 17]. However, in contrast to [15, 16, 17] our approach to the problem of PST does not rely on the concept of inverse eigenvalue problems, but rather on the derivation of Hamiltonians which lead to a particular transform namely, a permutation operation. Finally, the present work can also be viewed as an attempt to classify the Hamiltonian problems leading to exact revivals in discrete time evolution and the types of dynamics that appear during this evolution.

Our theoretical approach was also used for the derivation of Hamiltonians for the Fourier transform implemented using linear optical elements [19]. The general form of the Hamiltonian was given and the results are closely linked to the present ones as the Fourier transform is a cyclic operation (a property shown to be crucial for our considerations). The square of the Fourier transform gives a permutation operation, hence is related to the problem under investigation in the following sections.

The paper is organised as follows. In Sec. II we introduce our mathematical model and derive a class of Hamiltonians suitable for PST. In Sec. III, considering small networks we demonstrate how our theoretical approach can be used for quantum wire engineering. We show that certain Hamiltonians previously discussed in the literature are members of the larger unifying class derived in Sec. II. Moreover, we derive new PST Hamiltonians in the framework of NN-type, coulomb and dipole-dipole interactions. In Sec. IV, we analyse and discuss the dynamics induced by various types of PST Hamiltonians while we conclude with a summary of our main results in Sec. V.

II. HAMILTONIANS FOR PERFECT STATE TRANSFER

The model we consider is a network consisting of n sites labelled by $\{1, 2, \ldots, n\} \equiv \mathbb{S}_n$. At time $t = 0$, the qubit (e.g, spin) in the 1-st (input) site of the network is prepared in the state $|\psi_{\rm in}\rangle$. We wish to transfer to the n-th (output) site of the network with unit efficiency after a well defined period of time, let us say $t_{\rm r} \equiv \tau/J$, where J^{-1} is our time units ($\hbar = 1$).

We are interested in perfect passive quantum wires i.e., networks involving permanently coupled sites without any additional external control. Depending on the physical realization of the network, J can be a characteristic energy in our system, a coupling constant or tunnelling (hopping) rate, etc. Nevertheless, to present a generic theoretical approach to the problem of PST, the following discussion will be based on the dimensionless quantity τ. It is also worth noting, that τ need not always be a continuous variable as in some physical realizations (e.g., passive linear optical networks), the excitation (i.e., photon) evolves under successive applications of identical (practically instantaneous) unitary operations induced by the system's Hamiltonian [20]. In this case τ is simply the number of unitary operations we have applied. The subsequent discussion applies to all these physical realizations no matter whether they involve discrete or continuous evolution. However, for the sake of brevity we mainly refer to τ as number of applications (iterations) of identical unitary operations.

Our purpose is to explore the possible forms that the system's Hamiltonian $\mathcal{H}$ may take, to be suitable for PST. In other words, we wish to analyse the whole class of Hamiltonians $\mathfrak{C}_{\mathcal{H}}$, which lead to PST from the first to the last site after exactly τ applications. Following previous work in the field [10, 11, 12, 13, 14, 15, 16, 17, 18], we will assume that the network does not disturb the transmitted state and the main source of possible dissipation and decoherence is the fact that the wave packet (quantum information) spreads along the network. Hence, we are interested in Hamiltonians which preserve the total number of excitations in the system. For instance, in the framework of spin chains and arrays of quantum dots this means that the Hamiltonian commutes with the total spin operator [13, 14, 15, 16, 17, 18].

One way to guarantee all of these requirements is to concentrate our subsequent investigation on Hamiltonians for which the associated unitary evolution $\mathcal{U}$, leads to a permutation matrix after τ applications i.e.,

$$\mathcal{U}(\tau) \equiv e^{{\rm i}\mathcal{H}\tau} = \mathcal{P}, \tag{1}$$

where

$$\mathcal{P} = \begin{pmatrix} 0 & & \\ \vdots & \quad \tilde{\mathcal{P}} & \\ 0 & & \\ 1 & 0 \ \cdots \ 0 & \end{pmatrix}, \tag{2}$$

is a permutation in the single excitation sector i.e. also the submatrix $\tilde{\mathcal{P}}$ in the computational basis is a permutation. The permutation matrix (2) guarantees that the net effect of the evolution (1) is the transfer of the excitation from the first position to the last one i.e.,

$|1\rangle_1|0\rangle_2...|0\rangle_n \rightarrow |0\rangle_1|0\rangle_2...|1\rangle_n$. The condition (1) might seem restrictive at this point and this is in general indeed the case as one may derive Hamiltonians which satisfy the aforementioned requirements and do not lead to permutations, but rather to other unitary operations. Nevertheless, as we show later on, many known Hamiltonians suitable for PST are basically associated with permutations and can thus be obtained within the present unifying theoretical framework. Besides, we will demonstrate that we have infinitely many, yet unexplored, choices for quantum wire engineering which are not covered by previous work in the field. We have to point out, however, that condition (1) is indeed a severe restriction if one is interested only in perfect transfer of a particular set of possible states or properties of states such as probabilities, entanglement, etc.

Note now that perfect transfer of arbitrary single-qubit states is a sufficient condition for perfect transfer of arbitrary multi-qubit states. For instance, in this case the same perfect quantum wire can be used multiple times for the transfer of each qubit separately. Furthermore, as long as the number of excitations and the transmitted qubit state are preserved by the Hamiltonian, the total Hilbert space in the problem can be decomposed into subspaces and we can focus on the one-excitation subspace. The corresponding basis is denoted by $\{|\alpha\rangle \mid \alpha \in \mathbb{S}_n\}$ and indicates the presence of the excitation at the site α. Hence, the problem of the PST is essentially reduced to the perfect transfer of a single excitation initially located at the 1-st site i.e., $|\psi_{\text{in}}\rangle = |1\rangle$.

In general, we can define $(n-1)!$ different permutations of the form (2), we have $n-1$ free positions to fill, and for each one of these our purpose now is to construct the class of Hamiltonians satisfying Eq. (1) and thus are suitable for PST. We can distinguish between cases where $\mathcal{P}$ consists of one or more cycles. In the following, we are going to investigate the two cases separately but we will see that the latter reduces to the former one within each cycle.

A. One-cycle permutations

For n sites we have $(n-2)!$ possible one-cycle permutations. In particular, starting from the $n \times n$ permutation

$$\mathcal{P} = \begin{pmatrix} 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{3}$$

the other possible one-cycle permutations can be obtained by simply relabelling the $(n-2)$ intermediate sites $\{2,\ldots,n-1\}$. In the following we will derive our results for this particular matrix.

To determine the class of Hamiltonians $\mathfrak{C}_{\mathcal{H}}$ satisfying Eq. (1) for the permutation (3), we need to know the eigenvalues and eigenvectors of the operator $\mathcal{P}$. The spectrum σ consists of n different eigenvalues of the characteristic equation $\lambda^n = 1$ i.e.,

$$\sigma = \{\lambda_j \mid \lambda_i \neq \lambda_j \text{ for } i,j \in \mathbb{Z}_n\}, \tag{4}$$

where

$$\lambda_j = \exp\left(\mathrm{i}2\pi\frac{j}{n}\right) \quad \text{for} \quad j \in \mathbb{Z}_n, \tag{5}$$

and $\mathbb{Z}_n \equiv \{0,1,\ldots,n-1\}$. The corresponding normalised eigenvectors can be expanded in the computational basis $\{|\alpha\rangle \mid \alpha \in \mathbb{S}_n\}$ as follows

$$\left|y_{\lambda_j}\right\rangle = \frac{1}{\sqrt{n}}\sum_{\alpha\in\mathbb{S}_n}\lambda_j^{\alpha-1}|\alpha\rangle = \frac{1}{\sqrt{n}}\left(1,\lambda_j^1,\ldots,\lambda_j^{n-1}\right), \tag{6}$$

and thus the spectral representation of $\mathcal{P}$ is

$$\mathcal{P} = \sum_{\lambda_j\in\sigma}\lambda_j\left|y_{\lambda_j}\right\rangle\left\langle y_{\lambda_j}\right|. \tag{7}$$

Using Eqs. (5)-(7), it is straightforward to construct a first Hamiltonian which satisfies Eq. (1) and (3) as follows

$$H = \frac{1}{\tau}\sum_{\lambda_j\in\sigma}\arg(\lambda_j)\left|y_{\lambda_j}\right\rangle\left\langle y_{\lambda_j}\right| \tag{8}$$

where $\arg(\lambda_j)$ is the phase of the j-th eigenvalue λ_j. However, this is not the only Hamiltonian which leads to the permutation $\mathcal{P}$ after τ applications. Additionally, we may shift each eigenenergy of the Hamiltonian (8) by an arbitrary integer multiple of 2π obtaining

$$\begin{aligned}\mathcal{H}_{\mathbf{l}} &= \frac{1}{\tau}H + \sum_{\lambda_j\in\sigma}\frac{2\pi l_{\lambda_j}}{\tau}\left|y_{\lambda_j}\right\rangle\left\langle y_{\lambda_j}\right| \\ &= \frac{1}{\tau}\sum_{\lambda_j\in\sigma}\left[\arg(\lambda_j)+2\pi l_{\lambda_j}\right]\left|y_{\lambda_j}\right\rangle\left\langle y_{\lambda_j}\right|, \end{aligned} \tag{9}$$

with $\mathbf{l} \in \mathbb{Z}^n \equiv \{(l_{\lambda_0}, l_{\lambda_1},\ldots,l_{\lambda_{n-1}}) \mid l_{\lambda_j} \in \mathbb{Z}, j \in \mathbb{Z}_n\}$. Therefore the class of Hamiltonians satisfying Eq. (1) for the particular one-cycle permutation (3) is

$$\mathfrak{C}_{\mathcal{H}} = \{\mathcal{H}_{\mathbf{l}} \mid \mathbf{l} \in \mathbb{Z}^n\}, \tag{10}$$

with $\mathcal{H}_{\mathbf{l}}$ given by Eq. (9). Since the members of $\mathfrak{C}_{\mathcal{H}}$ are parameterised by the integer vector $\mathbf{l} \in \mathbb{Z}^n$, the class $\mathfrak{C}_{\mathcal{H}}$ consists of infinitely many Hamiltonians suitable for PST.

Note now that all the members of $\mathfrak{C}_{\mathcal{H}}$ are linear superpositions of the projectors onto the eigensubspaces of the permutation $\mathcal{P}$. More precisely, Eq. (9) can be also written as

$$\mathcal{H}_{\mathbf{E}} = \sum_{\lambda_j\in\sigma}\varepsilon_{\lambda_j}\left|y_{\lambda_j}\right\rangle\left\langle y_{\lambda_j}\right| \equiv \sum_{\lambda_j\in\sigma}\varepsilon_{\lambda_j}\Pi_{\lambda_j}, \tag{11}$$

where the *spectrum* (eigenenergy-vector) $\mathbf{E} \in \mathbb{R}^n \equiv \{(\varepsilon_{\lambda_0},\ldots,\varepsilon_{\lambda_{n-1}}) \mid \varepsilon_{\lambda_j} \in \mathbb{R}, j \in \mathbb{Z}_n\}$.

Using Eq. (6), we can express Eq. (11) in the computational basis as follows

$$\mathcal{H}_{\mathbf{E}} = \sum_{\alpha,\beta\in\mathbb{S}_n} \sum_{\lambda_j\in\sigma} \varepsilon_{\lambda_j} \lambda_j^{\alpha-\beta} \left|\alpha\right\rangle \left\langle\beta\right|, \tag{12}$$

which can be also written in the usual form

$$\mathcal{H}_{\mathbf{E}} = \mathcal{H}_{\mathbf{E}}^{(0)} + \mathcal{V}_{\mathbf{E}} \tag{13}$$

with the diagonal part

$$\mathcal{H}_{\mathbf{E}}^{(0)} = \sum_{\alpha\in\mathbb{S}_n} E_\alpha \left|\alpha\right\rangle \left\langle\alpha\right| \tag{14}$$

and the interaction

$$\mathcal{V}_{\mathbf{E}} = \sum_{\alpha\neq\beta\in\mathbb{S}_n} G(\alpha,\beta) \left|\alpha\right\rangle \left\langle\beta\right|. \tag{15}$$

Thereby, the energies and the couplings are given by

$$E_\alpha = \sum_{\lambda_j\in\sigma} \varepsilon_{\lambda_j}, \tag{16}$$

$$G(\alpha,\beta) = \sum_{\lambda_j\in\sigma} \varepsilon_{\lambda_j} \lambda_j^{\alpha-\beta}. \tag{17}$$

From Eq. (16), we see that Hamiltonians which are associated with permutation (3) and lead to PST may only correspond to networks involving the same energy level for all the sites.

The conditions under which Hamiltonians with NN interaction may lead to PST have been extensively discussed in the literature during the last years [10, 12, 13, 14, 15, 16]. Such NN-interaction Hamiltonians are typically tridiagonal in the computational basis i.e., we have $G(\alpha,\beta) = 0$, for all $\beta \notin \{\alpha, \alpha\pm 1\}$. However, according to the following theorem the class of Hamiltonians $\mathfrak{C}_{\mathcal{H}}$ we have derived here does not include NN-interaction Hamiltonians.

Theorem. *For networks of arbitrary dimension ($n > 2$), there exists no nearest-neighbour-interaction Hamiltonian satisfying condition (1) in the framework of permutation (3).*

Proof. According to Eq. (11) all the Hamiltonians which satisfy Eq. (1) with $\mathcal{P}$ given by Eq. (3) are linear superpositions of the projectors Π_j. Moreover, they can be decomposed as described in Eqs. (13)-(17). For a given dimension $n > 2$, let us now assume that there exists a set of eigenenergies $\mathbf{x} \in \mathbb{R}^n$ such that the corresponding Hamiltonian $\mathcal{H}_{\mathbf{x}}$ involves NN interaction. We are going to show that such a Hamiltonian does not exist (proof by contradiction).

We start with the general decomposition of the interaction term $\mathcal{V}_{\mathbf{x}}$ as

$$\mathcal{V}_{\mathbf{x}} = \mathcal{V}_{\mathbf{x}}^{(\mathrm{N})} + \mathcal{V}_{\mathbf{x}}^{(\not\mathrm{N})}, \tag{18}$$

where $\mathcal{V}_{\mathbf{x}}^{(\mathrm{N})}$ involves NN interaction i.e., $\beta = \alpha \pm 1$, while $\mathcal{V}_{\mathbf{x}}^{(\not\mathrm{N})}$ involves terms with $\beta \notin \{\alpha, \alpha\pm 1\}$. Our assumption about the existence of an NN-type Hamiltonian implies that the Hamiltonian is tridiagonal in the computational basis, i.e.,

$$\mathcal{V}_{\mathbf{x}}^{(\mathrm{N})} \neq 0 \quad \text{and} \quad \mathcal{V}_{\mathbf{x}}^{(\not\mathrm{N})} = 0. \tag{19}$$

From the second condition and Eq. (15) we have that $G(\alpha,\beta) = 0$, for all $\beta \notin \{\alpha, \alpha\pm 1\}$. However, since $G(\alpha,\beta)$ depend only on $\alpha-\beta$ we may obtain $n-2$ linear equations for variables x_j (see Eq. 17), namely $\Lambda\mathbf{x} = \mathbf{0}$ where

$$\Lambda = \begin{pmatrix} \lambda_0^2 & \lambda_1^2 & \cdots & \lambda_{n-1}^2 \\ \lambda_0^3 & \lambda_1^3 & \cdots & \lambda_{n-1}^3 \\ \vdots & & & \vdots \\ \lambda_0^{n-1} & \lambda_1^{n-1} & \cdots & \lambda_{n-1}^{n-1} \end{pmatrix}. \tag{20}$$

Note now that, in view of Eq. (5), the matrix (20) is (up to first two missing rows and normalisation) the usual Fourier transformation. Hence, $\mathrm{rank}(\Lambda) = n-2$, while two linear independent solutions can be chosen as $\tilde{\mathbf{x}}_1 = (1,\ldots,1)$ and $\tilde{\mathbf{x}}_2 = (\overline{\lambda}_0,\ldots,\overline{\lambda}_{n-1})$. Asking for a linear combination of $\tilde{\mathbf{x}}_1$ and $\tilde{\mathbf{x}}_2$ to be real (because this plays the role of eigenenergy vector) we find that the only acceptable solution is multiple of $(1,\ldots,1)$. However, one can see immediately from Eqs. (14) and (15), that such a spectrum can be associated only with the system involving no interaction between sites i.e.,

$$\mathcal{V}_{\mathbf{x}}^{(\mathrm{N})} = 0 \quad \text{and} \quad \mathcal{V}_{\mathbf{x}}^{(\not\mathrm{N})} = 0. \tag{21}$$

which contradicts our initial assumption (19) about NN interaction. □

Closing the section we would like to emphasise that the presented method (including the proof) applies also to all other one cycle permutations. The explicit results will differ from the presented ones only by the corresponding permutation of the labels.

B. Many-cycle permutations

In the case of permutations consisting of more than one cycle, the situation is slightly more complicated but the problem can be treated separately within each cycle along the lines of the previous section. More precisely, consider a cycle of length $d < n$. Such a cycle does not involve all the network sites but rather a subset of them $\mathbb{S}_d \subset \mathbb{S}_n$. Hence, the related eigenvalues are given by

$$\lambda_j = \exp\left(\mathrm{i}2\pi\frac{j}{d}\right) \quad \text{for} \quad j \in \mathbb{Z}_d, \tag{22}$$

while for the projections of the corresponding eigenvectors onto the computational basis $\{\left|\alpha\right\rangle \mid \alpha \in \mathbb{S}_n\}$ we have

$$\left\langle \alpha \middle| v_{\lambda_j}^{(k)} \right\rangle = \begin{cases} \lambda_j^{\alpha-1}/\sqrt{d} & \text{for } \alpha \in \mathbb{S}_d \\ 0 & \text{otherwise} \end{cases}. \tag{23}$$

As is apparent from Eq. (22) the spectrum σ of a many-cycle permutation is always degenerate since at least one of the eigenvalues (i.e., the eigenvalue for $j = 0$) appears as many times as the total number of cycles. Hence, the same degenerate eigenvalue λ_j corresponds to δ_{λ_j} distinct eigenvectors from different cycles. To this end, in Eq. (23) the eigenvectors are characterised by the additional superscript $k \in \{1, \ldots, \delta_{\lambda_j}\}$, where δ_{λ_j} is the degeneracy of the eigenvalue λ_j. For a given degenerate eigenvalue λ_j, let us also denote by $\mathcal{E}_{\lambda_j}$ the subspace spanned by the δ_{λ_j} distinct eigenvectors $\{|v_{\lambda_j}^{(k)}\rangle\}$.

In view of the degeneracy in the spectrum of a many-cycle permutation we have more freedom in the construction of Hamiltonians satisfying condition (1). Indeed, as described in Sec. II A, for such a construction we first of all need a basis of orthonormal eigenvectors. However, within each eigensubspace $\mathcal{E}_{\lambda_j}$ we can choose such an eigenbasis $\{|y_{\lambda_j}^{(k)}\rangle\}$ in many different ways, by constructing linear superpositions of $\{|v_{\lambda_j}^{(k)}\rangle\}$. Moreover, for each eigenvector $|y_{\lambda_j}^{(k)}\rangle$ we have the additional freedom to shift the phase of its eigenvalue by a multiple of 2π, as we did in Sec. II A. So, the class of PST Hamiltonians (10) has infinitely many members of the form

$$\begin{aligned} \mathcal{H}_{\mathbf{l}} &= \frac{1}{\tau} \sum_{\lambda_j} \sum_{k=1}^{\delta_{\lambda_j}} \left[\arg(\lambda_j) + 2\pi l_{\lambda_j}^{(k)} \right] \left| y_{\lambda_j}^{(k)} \right\rangle \left\langle y_{\lambda_j}^{(k)} \right| \\ &= \frac{1}{\tau} \sum_{\lambda_j} \sum_{k=1}^{\delta_{\lambda_j}} \varepsilon_{\lambda_j}^{(k)} \left| y_{\lambda_j}^{(k)} \right\rangle \left\langle y_{\lambda_j}^{(k)} \right|, \end{aligned} \tag{24}$$

where $\mathbf{l} \in \mathbb{Z}^n \equiv \{(l_{\lambda_0}^{(1)}, \ldots, l_{\lambda_0}^{(\delta_{\lambda_0})}; l_{\lambda_1}^{(1)}, \ldots, l_{\lambda_1}^{(\delta_{\lambda_1})}; \ldots) \,|\, l_{\lambda_j}^{(k)} \in \mathbb{Z}\}$. This is a straightforward generalisation of Eq. (9) to the case of degenerate eigenvalues.

C. Quantum wire engineering

So far we have seen that given a permutation matrix of a particular form one may easily derive the whole class of PST Hamiltonians which lead to the permutation under consideration. Hence, our method provides a way of quantum wire engineering in the sense that it enables us to construct possible PST Hamiltonians (i.e., to define energies and coupling strengths) which are implementable in a particular setup. The starting point is always the choice of the permutation which need not be always random, as various factors (such as topology of our network and type of interactions) may automatically fix our permutation matrix. For instance, in the case of a centrosymmetric network one has to focus on antidiagonal permutation matrices only while, according to the theorem of Sec. II A, NN-type Hamiltonians automatically exclude all one-cycle permutations.

Having fixed our permutation, the construction of a PST Hamiltonian proceeds in two steps. In the first step one has to define the corresponding class of PST Hamiltonians working along the lines of this section. The members of this class are parameterised by a number of free parameters. In the second step one can estimate all these parameters by applying certain constraints based on the topology of the network as well as the form of the physical interactions implementable within the framework of a particular setup. This engineering process can be always performed numerically but in certain cases (especially for relatively small networks) derivation of analytic solutions might be possible. In the following section we discuss the quantum wire engineering in detail by explicitly constructing PST Hamiltonians for small networks.

III. EXAMPLES OF PST HAMILTONIANS

Let us devote some attention to the application of the proposed quantum wire engineering method to few concrete examples. Among the simplest we can think of, is the example of a small networks consisting of just few sites.

A. Nearest-neighbour interaction

Following the notation introduced in the previous section, we start with the investigation of the whole class of NN-type PST Hamiltonians in the context of a small network consisting of four sites only. The problem of PST in such a small network is amenable to analytic solutions thus offering the appropriate theoretical framework to demonstrate the application of our method.

We can define six 4×4 permutation matrices of the form (2) that is, two one-cycle permutations and four permutations involving more than one cycles. As we showed in the previous section, NN-type Hamiltonians cannot be obtained in the context of one-cycle permutations. Hence, for the purposes of this particular example, it is sufficient to restrict ourselves to permutation matrices involving more than one cycles only.

Let us consider first the antidiagonal permutation matrix

$$\mathcal{P}_4 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{25}$$

This permutation involves two cycles of dimension $d = 2$ namely, $\mathcal{C}_1 = (1, 4)$ and $\mathcal{C}_2 = (2, 3)$ [22]. Hence, according to Eq. (22) we have two eigenvalues $\lambda_0 = e^{\mathrm{i}0} = +1$ and $\lambda_1 = e^{\mathrm{i}\pi} = -1$. Both eigenvalues ± 1 are doubly degenerate (i.e., $\delta_\pm = 2$) and the corresponding eigenvectors are given by $|v_\pm^{(1)}\rangle = (|1\rangle \pm |4\rangle)/\sqrt{2}$ and $|v_\pm^{(2)}\rangle = (|2\rangle \pm |3\rangle)/\sqrt{2}$, for cycles $\mathcal{C}_1$ and $\mathcal{C}_2$, respectively. Accordingly, the corresponding subspaces are

$$\mathcal{E}_\pm = \left\{ \left| v_\pm^{(1)} \right\rangle, \left| v_\pm^{(2)} \right\rangle \right\}.$$

Having defined the permutation matrix, the construction of PST Hamiltonians now proceeds in two steps.

1. Step 1 — Parameterisation.

For each one of the subspaces we can choose an orthonormal basis in many different ways. For example, taking into account the orthogonality condition, we may choose for the two subspaces

$$\mathcal{E}_+ : \begin{cases} \left|y_+^{(1)}\right\rangle = \nu \left|v_+^{(1)}\right\rangle + \mu \left|v_+^{(2)}\right\rangle \\ \left|y_+^{(2)}\right\rangle = \mu^* \left|v_+^{(1)}\right\rangle - \nu^* \left|v_+^{(2)}\right\rangle, \end{cases} \tag{26}$$

and

$$\mathcal{E}_- : \begin{cases} \left|y_-^{(1)}\right\rangle = \xi \left|v_-^{(1)}\right\rangle + \zeta \left|v_-^{(2)}\right\rangle \\ \left|y_-^{(2)}\right\rangle = \zeta^* \left|v_-^{(1)}\right\rangle - \xi^* \left|v_-^{(2)}\right\rangle. \end{cases} \tag{27}$$

Thereby, $\mu, \nu, \xi, \zeta \in \mathbb{C}$ such that

$$|\mu|^2 + |\nu|^2 = 1 \quad \text{and} \quad |\xi|^2 + |\zeta|^2 = 1. \tag{28}$$

According to the theory of the previous section, the corresponding eigenergies can be chosen as

$$\mathcal{E}_+ : \begin{cases} \varepsilon_+^{(1)} = 0 + 2\pi l_+^{(1)} \\ \varepsilon_+^{(2)} = 0 + 2\pi l_+^{(2)}, \end{cases} \tag{29}$$

and

$$\mathcal{E}_- : \begin{cases} \varepsilon_-^{(1)} = \pi + 2\pi l_-^{(1)} \\ \varepsilon_-^{(2)} = \pi + 2\pi l_-^{(2)}, \end{cases} \tag{30}$$

for $l_j^{(k)} \in \mathbb{Z}$. Thereby, note that the eigenvalues of subspace $\mathcal{E}_+$ ($\mathcal{E}_-$) are even (odd) integer multiples of π.

Thus, the whole class of PST Hamiltonians (24) reads

$$\begin{aligned} \mathcal{H}_{\mathbf{1}}^{(4)} \;=\; \frac{1}{\tau}\Big[& \varepsilon_+^{(1)} \left|y_+^{(1)}\right\rangle \left\langle y_+^{(1)}\right| + \varepsilon_+^{(2)} \left|y_+^{(2)}\right\rangle \left\langle y_+^{(2)}\right| \\ & + \varepsilon_-^{(1)} \left|y_-^{(1)}\right\rangle \left\langle y_-^{(1)}\right| + \varepsilon_-^{(2)} \left|y_-^{(2)}\right\rangle \left\langle y_-^{(2)}\right| \Big], \end{aligned} \tag{31}$$

with open parameters the spectrum $\{\varepsilon_+^{(1)}, \varepsilon_+^{(2)}, \varepsilon_-^{(1)}, \varepsilon_-^{(2)}\}$ [or equivalently the integers $l_\pm^{(1,2)}$] and two independent complex numbers (due to normalisation), say μ and ξ. As we discuss in the following subsection, all these parameters can be specified by imposing additional constraints on the form of the resulting Hamiltonian. Moreover, we would like to note that, due to the form of the eigenvectors, all the members of this class are symmetric along the diagonal and the antidiagonal.

2. Step 2 — Parameter estimation.

Assume now that we are interested in the whole class of NN-type Hamiltonians leading to the antidiagonal permutation matrix (25) and are of the form

$$\mathcal{H}^{(4)} = \begin{pmatrix} E_1 & g_1 & 0 & 0 \\ g_1 & E_2 & g_2 & 0 \\ 0 & g_2 & E_2 & g_1 \\ 0 & 0 & g_1 & E_1 \end{pmatrix}. \tag{32}$$

Since the class (31) has been derived within a rather general framework (limited only by the particular form of the permutation), our task reduces to the application of specific constraints on the parameters entering $\mathcal{H}_{\mathbf{1}}^{(4)}$.

We will focus on the case of Hamiltonians with non-degenerate spectrum i.e., all the eigenenergies $\varepsilon_\pm^{(1,2)}$ are different. The case of degenerate spectrum can be treated similarly and leads to NN-type Hamiltonians with vanishing couplings. Hence, such solutions correspond to a broken network and can never lead to PST from the first to the last site.

Rewriting Eq. (31) in the computational basis and asking for Hamiltonians of the form (32), we have that the matrix elements $\langle 1| \mathcal{H}_{\mathbf{1}}^{(4)} |3\rangle$ and $\langle 1| \mathcal{H}_{\mathbf{1}}^{(4)} |4\rangle$ must vanish. Thus we obtain the following set of nontrivial constraints on the free parameters,

$$\varepsilon_+^{(1)}|\nu|^2 + \varepsilon_+^{(2)}|\mu|^2 - \varepsilon_-^{(1)}|\xi|^2 - \varepsilon_-^{(2)}|\zeta|^2 = 0, \tag{33a}$$

$$(\varepsilon_+^{(1)} - \varepsilon_+^{(2)})\nu\mu^* + (\varepsilon_-^{(2)} - \varepsilon_-^{(1)})\xi\zeta^* = 0. \tag{33b}$$

Other equations which can be obtained from the remaining matrix elements $\langle i| \mathcal{H}_{\mathbf{1}}^{(4)} |j\rangle$ will be used later on, for the derivation of sets $\{E_1, E_2\}$ and $\{g_1, g_2\}$ for which the Hamiltonian (32) enables PST.

Using the normalisation conditions (28), Eq. (33a) can be also expressed in terms of differences of eigenvalues only i.e.,

$$(\varepsilon_+^{(1)} - \varepsilon_+^{(2)})|\nu|^2 - (\varepsilon_-^{(1)} - \varepsilon_-^{(2)})|\xi|^2 + \varepsilon_+^{(2)} - \varepsilon_-^{(2)} = 0.$$

This fact indicates that the existence of a solution to the problem of PST depends mainly on differences of eigenenergies. In other words, if we have a solution for a particular choice of the spectrum, say $\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4\}$, then there also exist the solutions for all the spectra of the form $\{\varepsilon_1 + 2\pi j, \varepsilon_2 + 2\pi j, \varepsilon_3 + 2\pi j, \varepsilon_4 + 2\pi j\}$ with $j \in \mathbb{Z}$.

Assume now that ν and ξ are real and non-negative. Such an assumption is not restrictive because the global phase of each eigenvector can be chosen arbitrarily without changing the Hamiltonian (and thus dynamics). The phases of μ and ζ will be denoted by φ and χ, respectively. Solving Eqs. (33) with the normalisation conditions (28), we obtain for the absolute values of the pa-

rameters μ, ν, ξ, and ζ

$$
\begin{aligned}
|\mu| &= \sqrt{\frac{(\varepsilon_+^{(2)}-\varepsilon_-^{(2)})(\varepsilon_-^{(1)}-\varepsilon_+^{(2)})}{(\varepsilon_+^{(1)}-\varepsilon_+^{(2)})(\varepsilon_+^{(1)}-\varepsilon_-^{(2)}-\varepsilon_-^{(1)}+\varepsilon_+^{(2)})}},\\
|\nu| &= \sqrt{\frac{(\varepsilon_-^{(1)}-\varepsilon_+^{(1)})(\varepsilon_-^{(2)}-\varepsilon_+^{(1)})}{(\varepsilon_+^{(1)}-\varepsilon_+^{(2)})(\varepsilon_+^{(1)}-\varepsilon_-^{(2)}-\varepsilon_-^{(1)}+\varepsilon_+^{(2)})}},\\
|\xi| &= \sqrt{\frac{(\varepsilon_-^{(2)}-\varepsilon_+^{(1)})(\varepsilon_-^{(2)}-\varepsilon_+^{(2)})}{(\varepsilon_-^{(1)}-\varepsilon_-^{(2)})(\varepsilon_+^{(1)}-\varepsilon_-^{(2)}-\varepsilon_-^{(1)}+\varepsilon_+^{(2)})}},\\
|\zeta| &= \sqrt{\frac{(\varepsilon_-^{(1)}-\varepsilon_+^{(1)})(\varepsilon_-^{(1)}-\varepsilon_+^{(2)})}{(\varepsilon_-^{(2)}-\varepsilon_-^{(1)})(\varepsilon_+^{(1)}-\varepsilon_-^{(2)}-\varepsilon_-^{(1)}+\varepsilon_+^{(2)})}}. \quad (34)
\end{aligned}
$$

Moreover, from Eq. (33b) we have that a solution exists if and only if the phases of the amplitudes satisfy the relation

$$\varphi - \chi = m\pi, \quad m \in \mathbb{Z} \tag{35}$$

where m must be odd(even) for $(\varepsilon_+^{(1)}-\varepsilon_+^{(2)})/(\varepsilon_-^{(1)}-\varepsilon_-^{(2)})$ negative(positive), respectively. Finally, it is straightforward to show that the normalisation condition and the non-negativity of the right-hand sides in Eqs. (34) imply that the intervals between $\left[\varepsilon_+^{(1)},\ \varepsilon_+^{(2)}\right]$ and $\left[\varepsilon_-^{(1)},\ \varepsilon_-^{(2)}\right]$ must overlap but need not be one inside the other. For instance, one can readily check that the spectra discussed in many papers [13, 14, 15, 16] fulfil this condition and thus can be obtained within the present formalism. We have also verified this fact numerically for larger networks.

At this point, we have analysed completely the PST Hamiltonians which lead to the permutation matrix (25). Indeed, using the expressions for the absolute values and choosing the phases and the spectra according to the aforementioned constraints, it is straightforward to derive possible combinations of $\{E_1, E_2\}$ and $\{g_1, g_2\}$ which lead to PST transfer by means of the equations

$$\langle 1|\,\mathcal{H}_{\mathbf{1}}^{(4)}\,|1\rangle = E_1, \quad \langle 2|\,\mathcal{H}_{\mathbf{1}}^{(4)}\,|2\rangle = E_2,$$

and

$$\langle 1|\,\mathcal{H}_{\mathbf{1}}^{(4)}\,|2\rangle = g_1, \quad \langle 2|\,\mathcal{H}_{\mathbf{1}}^{(4)}\,|3\rangle = g_2,$$

respectively.

The remaining question is whether there are other 4×4 many-cycle permutation matrices generated by NN-type Hamiltonians. To answer, we have to analyse the three remaining configurations of cycles.

- Permutation $(4,1)(2)(3)$. In this case we have two cycles of lengths two, one, and one, respectively and two different eigenvalues namely, $+1$ (degeneracy $\delta_{+1}=3$) and -1. Following the theory of Sec. II B and working as before for the subspace $\mathcal{E}_+$, we can define new eigenvalues $\varepsilon_+^{(i)} = 2\pi l_+^{(i)}$ with the corresponding eigenvectors in the computational basis given by $|y_+^{(i)}\rangle = \mu_i(|1\rangle + |4\rangle)/\sqrt{2} + \nu_i\,|2\rangle + \xi_i\,|3\rangle$, for $i \in \{1,2,3\}$. In the subspace $\mathcal{E}_-$, the eigenvalue and the eigenvector remain unchanged i.e., $\varepsilon_- = -1$ and $|y_-\rangle = (|1\rangle - |4\rangle)/\sqrt{2}$. Hence, the general form of the Hamiltonian which leads to the permutation under consideration after τ applications is given by

$$\tilde{\mathcal{H}}_{\mathbf{1}}^{(4)} = \frac{1}{\tau}\left[\sum_{i=1}^{3}\varepsilon_+^{(i)}\left|y_+^{(i)}\right\rangle\left\langle y_+^{(i)}\right| + \varepsilon_-\,|y_-\rangle\,\langle y_-|\right].$$

  Recall now that we are interested only in NN-type Hamiltonians i.e., Hamiltonians with $\langle 4|\,\tilde{\mathcal{H}}_{\mathbf{1}}^{(4)}\,|2\rangle = 0$ and $\langle 1|\,\tilde{\mathcal{H}}_{\mathbf{1}}^{(4)}\,|3\rangle = 0$. Rewriting $\tilde{\mathcal{H}}_{\mathbf{1}}^{(4)}$ in the computational basis, we find that these two conditions also imply $\langle 1|\,\tilde{\mathcal{H}}_{\mathbf{1}}^{(4)}\,|2\rangle = 0$ and $\langle 4|\,\tilde{\mathcal{H}}_{\mathbf{1}}^{(4)}\,|3\rangle = 0$. In other words, the first and the last sites are completely decoupled from their respective neighbours and thus there are no NN-type Hamiltonians which lead to PST in the context of the permutation $(4,1)(2)(3)$. Strictly speaking, PST from the first to the last site may occur only if these two sites are directly coupled. This is, however, the case of a trivial two-site network for which PST is always possible.

- Permutation $(4,1,3)(2)$. In this case we have two cycles of lengths three and one, respectively. The general form of eigenvectors in the computational basis is $|y_+^{(1)}\rangle = \mu(|1\rangle + |3\rangle + |4\rangle)/\sqrt{3} + \nu\,|2\rangle$ and $|y_+^{(2)}\rangle = -\nu^*(|1\rangle+|3\rangle+|4\rangle)/\sqrt{3}+\mu^*\,|2\rangle$ for the eigenvalue $+1$, $|y_x\rangle = (|1\rangle + x\,|3\rangle + x^2\,|4\rangle)/\sqrt{3}$ for the eigenvalue x, and $|y_{x^2}\rangle = (|1\rangle + x^2\,|3\rangle + x\,|4\rangle)/\sqrt{3}$ for the eigenvalue x^2, where $x = \exp(2i\pi/3)$. Asking for a NN-type Hamiltonian, among others, we obtain the constraints

$$
\begin{aligned}
\varepsilon_{+1}^{(1)}|\mu|^2 + \varepsilon_{+1}^{(2)}|\nu|^2 + \varepsilon_x x + \varepsilon_{x^2}x^2 = 0,\\
\varepsilon_{+1}^{(1)}|\mu|^2 + \varepsilon_{+1}^{(2)}|\nu|^2 + \varepsilon_x x^2 + \varepsilon_{x^2}x = 0,
\end{aligned}
$$

  which should be satisfied simultaneously. This implies the condition $(\varepsilon_x - \varepsilon_{x^2})(x - x^2) = 0$ which cannot be fulfiled because ε_x and ε_{x^2} are of the form $\varepsilon_x = (2/3 + 2l_3)\pi$, and $\varepsilon_{x^2} = (4/3 + 2l_4)\pi$, with $l_3, l_4 \in \mathbb{Z}$.

- Permutation $(4,1,2)(3)$. This case is similar to the permutation $(4,1,3)(2)$.

Hence, for the four-site network, NN-type PST Hamiltonians involving permutation transformation can be obtained only in the framework of the antidiagonal permutation matrix (25).

Concluding this simple example it is worth keeping in mind the aforementioned observation about the overlap of the intervals for odd and even eigenvalues. This turns out to be a particularly useful result as it enables us to

construct more PST Hamiltonians by changing appropriately the spectrum of an already known PST Hamiltonian. Most importantly, we have verified numerically the functionality of this idea for interactions beyond nearest neighbours and for networks involving more than four sites (e.g., see Table I in the next example). We turn now to discuss PST Hamiltonians beyond NN interaction.

B. Beyond nearest-neighbour interaction

In the previous example we explicitly discussed the construction of NN-type PST Hamiltonians. In [17] the problem of PST Hamiltonians beyond NN interaction was addressed for the first time. Motivated by this work we have studied the problem of PST Hamiltonians with a prescribed drop off of the coupling constants also in our theoretical framework. In this case, naturally, we do have only a very limited control over the form of the Hamiltonian. However, before we proceed to present related results, we point out that the class of Hamiltonians derived in Sec. II A is already of the beyond nearest neighbour type.

We have applied our method to Hamiltonians involving two different types of interactions and for networks with a moderate number of sites namely, four and six. For the latter case we present some of the obtained numerical results. Consider the Hamiltonian of the form

$$\mathcal{H}^{(6)} = \begin{pmatrix} E_1 & \frac{1}{r_1^\gamma} & \frac{1}{(r_1+r_2)^\gamma} & \frac{1}{(r_1+r_2+r_3)^\gamma} & \frac{1}{(r_1+2r_2+r_3)^\gamma} & \frac{1}{(2r_1+2r_2+r_3)^\gamma} \\ \frac{1}{r_1^\gamma} & E_2 & \frac{1}{r_2^\gamma} & \frac{1}{(r_2+r_3)^\gamma} & \frac{1}{(2r_2+r_3)^\gamma} & \frac{1}{(r_1+2r_2+r_3)^\gamma} \\ \frac{1}{(r_1+r_2)^\gamma} & \frac{1}{r_2^\gamma} & E_3 & \frac{1}{r_3^\gamma} & \frac{1}{(r_2+r_3)^\gamma} & \frac{1}{(r_1+r_2+r_3)^\gamma} \\ \frac{1}{(r_1+r_2+r_3)^\gamma} & \frac{1}{(r_2+r_3)^\gamma} & \frac{1}{r_3^\gamma} & E_3 & \frac{1}{r_2^\gamma} & \frac{1}{(r_1+r_2)^\gamma} \\ \frac{1}{(r_1+2r_2+r_3)^\gamma} & \frac{1}{(2r_2+r_3)^\gamma} & \frac{1}{(r_2+r_3)^\gamma} & \frac{1}{r_2^\gamma} & E_2 & \frac{1}{r_1^\gamma} \\ \frac{1}{(2r_1+2r_2+r_3)^\gamma} & \frac{1}{(r_1+2r_2+r_3)^\gamma} & \frac{1}{(r_1+r_2+r_3)^\gamma} & \frac{1}{(r_1+r_2)^\gamma} & \frac{1}{r_1^\gamma} & E_1 \end{pmatrix}. \quad (36)$$

which refers to a network where interactions extend beyond nearest neighbours and drop off with distance as $1/r^\gamma$. Our purpose is to find combinations of energies $\{E_1, E_2, E_3\}$ and distances $\{r_1, r_2, r_3\}$, such that $\mathcal{H}^{(6)}$ leads to an antidiagonal 6×6 permutation matrix after precisely τ applications.

As in the previous example, the Hamiltonian design proceeds in two steps. First we have to find a general parameterisation of the possible PST Hamiltonians along the lines of Sec. II B. Subsequently, asking for Hamiltonians of the form (36), we obtain a set of equations for the free parameters entering our design. This system of equations can be solved by means of standard numerical techniques yielding a number of acceptable solutions (i.e., sets of energies $\{E_1, E_2, E_3\}$ and distances $\{r_1, r_2, r_3\}$). A few of them, for the coulomb ($\gamma = 1$) and the dipole-dipole ($\gamma = 3$) interaction are given in Table I. In discussing this table, we would like to note that the solution (a) for the dipole-dipole interaction coincides (apart from a shift in the energies) with the one given by Kay [17], while all the other solutions are new and have not been discussed in the literature before. Moreover, as is evident from the table footnotes, for both solutions (a) and (b) we have an overlap of the spectrum for even and odd eigenvalues. More solutions can be obtained in a straightforward manner by modifying appropriately these spectra, while they overlap.

Throughout this section, for the sake of simplicity and illustration, we have focused on small networks and particular choices of Hamiltonians. In closing we would like to emphasise that the presented solutions are by no means exhaustive. Our theoretical approach to the problem of PST is able to provide infinitely many solutions and is not *a priori* restricted to particular topologies and/or coupling configurations. In the following section we turn to discuss the evolution of the excitation under the influence of various types of PST Hamiltonians.

TABLE I: Perfect state transfer. Parameters entering the Hamiltonian (36), for $\gamma = 1$ (Coulomb interaction) and $\gamma = 3$ (dipole-dipole interaction). The depicted values for the energies and the distances should be multiplied by π/τ and $(\tau/\pi)^{1/\gamma}$, respectively.

	Coulomb interaction		Dipole interaction	
Parameter	Solution[a]	Solution[b]	Solution[a]	Solution[b]
E_1	1.07571	1.10848	-0.00885	0.36328
E_2	-0.70069	-0.73164	-0.61799	-1.89782
E_3	-1.87501	-3.87684	-0.87315	-1.96546
r_1	1.77185	1.93029	0.96704	0.97927
r_2	1.12358	0.71338	0.90156	0.74773
r_3	0.96133	1.06286	0.88587	0.89090

[a] Eigenenergies: $\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6\} = \{2, 0, -2, -1, -3, 1\}$.
[b] Eigenenergies: $\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6\} = \{2, 0, -4, -1, -5, 1\}$.

IV. WAVE PACKET DYNAMICS

The Hamiltonians given in the previous sections are quite abstract. To illustrate in more detail the dynamics they can induce we present a few examples of how the dynamics of a single excitation will look like. In particular we will comment on two parameters namely the occupation probability distribution and the corresponding entanglement. As we mentioned before, there are infinitely many PST Hamiltonians one may propose, and each one of them may induce a new type of dynamics. Hence, the patterns we have chosen to discuss in this section at any rate cannot be considered as representatives of the whole range of patterns generated by all the possible PST Hamiltonians.

A. Occupation probability distribution

In Sec. II we have explicitly constructed the whole class of Hamiltonians $\mathfrak{C}_{\mathcal{H}}$ which satisfy condition (1). In particular, we have seen that there are infinitely many Hamiltonians $\mathcal{H}_{\mathbf{l}}$ which in general may lead to different evolution operators and thus to different dynamics. A more detailed classification is not an easy task. Nevertheless, in this section we discuss typical transfer dynamics associated with particular choices of the spectrum, or equivalently the integer vector $\mathbf{l}$ entering the members of $\mathfrak{C}_{\mathcal{H}}$.

An excitation initially localized at site i evolves under m applications of the Hamiltonian (24) according to

$$\begin{aligned}\mathcal{U}_{\mathbf{l}}(m)\,|i\rangle &\equiv e^{\mathrm{i}\mathcal{H}_{\mathbf{l}}m}\,|i\rangle \\ &= \sum_{\lambda_j\in\sigma}\sum_{k=0}^{\delta_{\lambda_j}}\exp\left(\mathrm{i}\varepsilon_{\lambda_j}^{(k)}m\right)|y_{\lambda_j}^{(k)}\rangle\langle y_{\lambda_j}^{(k)}|i\rangle.\end{aligned} \tag{37}$$

The corresponding probability to find the excitation at site f is given by

$$\begin{aligned}P_f(m) &\equiv \langle f|\,\mathcal{U}_{\mathbf{l}}(m)\,|i\rangle \\ &= \left|\sum_{\lambda_j\in\sigma}\sum_{k=0}^{\delta_{\lambda_j}}\exp\left(\mathrm{i}\varepsilon_{\lambda_j}^{(k)}m\right)\langle f|y_{\lambda_j}^{(k)}\rangle\langle y_{\lambda_j}^{(k)}|i\rangle\right|^2.\end{aligned} \tag{38}$$

Hence, during the transfer the probability of finding the excitation may spread among all the sites of the network which become essentially entangled. However, no matter how complicated the transfer dynamics may be, we have the desired perfect transfer of the excitation after exactly τ applications since $\mathcal{U}_{\mathbf{l}}(\tau)=\mathcal{P}$.

Let us have a more detailed look at the single excitation (e.g., photon) wave packet dynamics, initially localised at the first site i.e., $|i\rangle=|1\rangle$ in Eq. (38). In Fig. 1 we plot the evolution of the occupation probability distribution as a function of the number of applications m, for a medium size network of 11 sites (modes). The four plots differ by the choice of the spectrum. More precisely, the first plot has been obtained for the spectrum with $l_{\lambda_j}=11-j$, the second plot is for the spectrum with $l_{\lambda_{2j-1}}=19-3j$ and $l_{\lambda_{2j}}=0$ (for $1\leq j\leq 6$), and the third plot corresponds to the symmetric spectrum with $l_{\lambda_j}=|j-6|$. The last plot corresponds to an alternating sequence of eigenenergies with $l_{\lambda_{4j-3}}=l_{\lambda_{4j-2}}=0$, and $l_{\lambda_{4j-1}}=l_{\lambda_{4j}}=5$, for $1\leq j\leq 3$.

The descendent sequence of eigenvalues used in Fig. 1(a) results in a gradual transfer of the excitation from the initial position to the target position. At each iteration instant the wave packet is slightly shifted and only few of the adjacent modes is noticeable excited. On the contrary, for all the other plots the wave packet is not only broadened and propagating, but splits into two or more components. As a result there is a nonzero probability to detect the excitation at two or more distant sites at specific instances of the evolution. In particular, when the decreasing sequence of eigenvalues is interrupted by zero values, the probability distribution pattern is formed by several "paths" which transfer the initial excitation to the final target site [see Fig. 1(b)]. When the eigenvalue sequence exhibits a symmetric dip, the probability distribution is formed by two intersecting lines along which the probability propagates [see Fig. 1(c)]. The final plot [Fig. 1(d)], applicable for the tooth like sequence of eigenvalues, shows an effective transfer of probability along the outer parts of the network. The central modes [23] are never significantly populated during the wave packet propagation.

B. Entanglement

The behaviour of the single excitation (e.g., photon) in a network implementing PST can be discussed also from the point of view of entanglement. We can ask how the propagation of the photon in different types of networks affects the mutual (bipartite) entanglement. The bipartite entanglement can be quantified using the concept of concurrence [21]. For the single photon excitation the bipartite entanglement between two selected modes, say i and j, is given by [20]

$$C_{ij}(m)=2\sqrt{P_i(m)P_j(m)}.$$

This simple result shows that shaping the probability distribution strongly influences the entanglement properties. The more the photon spreads across the modes during the evolution the more entangled the modes become. When analysing the bipartite entanglement between the initial mode and the remaining modes we find that the entanglement plots exhibit a very similar structure to the one of the probability distribution shown in Figs. 1(a-d). The main difference is that, due to the probability multiplication in the definition of the concurrence, the peaks become broader and less pronounced.

Due to the similarity we do not present any plots regarding the bipartite entanglement. Instead, we proceed to discuss the single-excitation dynamics from the point of view of the overall bipartite entanglement $T(m)$, where additional conclusions can be drawn.

By definition, $T(m)$ is the sum of all C_{ij}^2 and is given by[20]

$$T(m) = 2\left[1 - \sum_i P_i(m)^2\right].$$

Therefore, we see that the overall bipartite entanglement after m applications of the Hamiltonian is specified by the squared probabilities (essentially the purity – linearised entropy related to the probability distribution). The more localized the distribution is, the less overall bipartite entanglement the propagating wave pattern contains. In particular for the patterns presented in Figs. 1(a-d) we come to the following conclusions concerning the overall bipartite entanglement.

The choice of the spectra influences the maximum value of T which can be attained during the propagation as well as its modulation. As is depicted in Fig. 2, the overall bipartite entanglement for the monotonously decreasing [Fig. 2(a)] and the symmetric-dip spectrum [Fig. 2(c)] exhibits simple forms. In both cases the excitation occupies at least one of the intermediate sites with probability one [see Figs. 1(a), (c) respectively] and this fact is reflected in T which drops to zero.

The overall bipartite entanglement for the two other spectra acquires a more complicated structure and the maximum value of T in Fig. 2(b) comes rather close to the maximum achievable value of 1.81 [20]. This just indicates that the wave packet is quite uniformly distributed among the sites [see Fig. 1(b),(d)]. The question whether the prescribed maximum can be indeed reached by some Hamiltonian for any of the classes we have discussed throughout this work is not difficult to answer. It is sufficient to take as an example the Hamiltonian inducing the Fourier transform. This transform is cyclic and its square leads to a permutation matrix, hence is among the Hamiltonians described by our method. At prescribed instances it distributes the excitation uniformly among the sites and hence will saturate T for any number of sites.

V. CONCLUSIONS

We analysed the problem of PST through passive networks(channels) and the Hamiltonians which induce the corresponding transform. The transform is represented by a permutation matrix which has particularly simple algebraic properties. Hence, in the case of one-cycle permutations we were able to obtain closed expressions for the whole class of NN-type Hamiltonians, while we proved that there exists no PST Hamiltonian in the framework of NN interactions. In the case of many-cycle permutations, the situation is more involved and for the time being the derivation of analytic expressions seems to by possible only in the case of relatively small networks. However, at any rate the problem can be still treated numerically.

In contrast to previous work in the field, our theory is not limited by any *a priory* restrictions to the topology of the system and the configuration of couplings between different sites of the network. Hence, our approach provides new ways for quantum wire engineering for systems of arbitrary topology and interactions. In this spirit, we were able on the one hand to recover all the known types of PST Hamiltonians restricted to centrosymmetric networks and/or NN interaction, and on the other hand to derive new Hamiltonians. In principle there are infinitely many PST Hamiltonians which can be described within our theoretical framework. However, we would like to emphasise that the different types of Hamiltonians need not be always implementable by a specific experimental setup. Actually, which types of Hamiltonians are indeed implementable has to be decided on the basis of the types of the particular physical interactions used in the system. Finally, apart from studying the form of PST Hamiltonians we also discussed the dynamics induced by them in terms of occupation probability distribution and overall bipartite entanglement.

Additional interesting questions linked to the present problem such as, stability of the Hamiltonians with respect to coupling constant perturbation, detailed analysis of the structure of the permutation cycles and the form of corresponding Hamiltonians, generalisations to higher dimensions etc, are left for further investigation.

VI. ACKNOWLEDGEMENT

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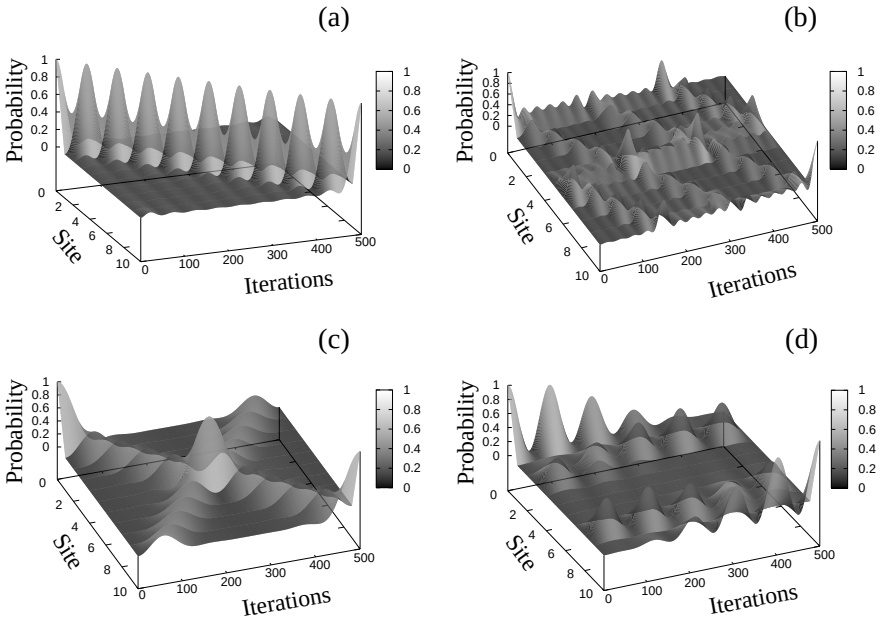

FIG. 1: Evolution of the occupation probability distribution governed by PST Hamiltonians of various spectra. Each plot corresponds to a network of eleven sites and 500 successive applications of the corresponding PST Hamiltonian. While the monotonously d ıduce more complicated pat ıs sites, the wave packet can

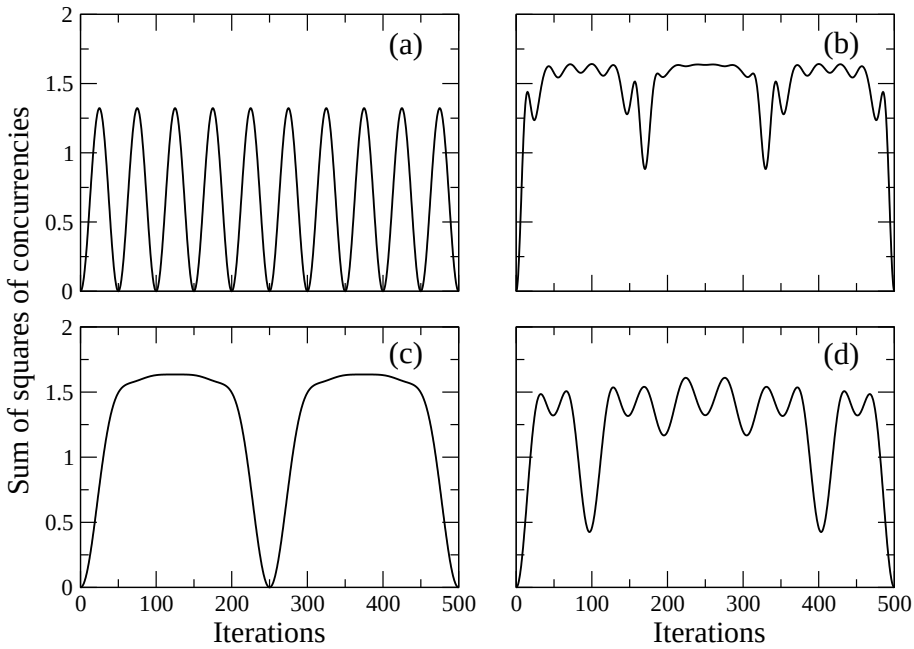

FIG. 2: Evolution of the overall concurrence corresponding to Figs. 1(a)-(c), as a function of iterations.

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[22] Thereby the notation $(2, 3)$ means that starting from the original site ordering $\{1, 2, 3, 4\}$, the second site is replaced by the third and the third site by the second.
[23] When referring to "central modes" we do not refer to the topology of the network but rather to the ordering of the computational basis states.